

Spin dependent transport of “nonmagnetic metal/zigzag nanotube encapsulating magnetic atoms/nonmagnetic metal” junctions

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Abstract

Towards a novel magnetoresistance (MR) device with a carbon nanotube, we propose “nonmagnetic metal/zigzag nanotube encapsulating magnetic atoms/nonmagnetic metal” junctions. We theoretically investigate how spin-polarized edges of the nanotube and the encapsulated magnetic atoms influence on transport. When the on-site Coulomb energy divided by the magnitude of transfer integral, $U/|t|$, is larger than 0.8, large MR effect due to the direction of spins of magnetic atoms, which has the magnitude of the MR ratio of about 100%, appears reflecting such spin-polarized edges.

Key words: Greens function method; magnetotransport

1. Introduction

Spin dependent transport of junctions with a carbon nanotube [1,2,3,4,5,6,7] is one of the most interesting topics in nano-spintronics fields. In fact, since it was reported that ferromagnet (FM)/carbon nanotube/FM junctions exhibited the magnetoresistance (MR) effect [8] with the magnitude of the MR ratio of 9% at 4.2 K [1], many experimental and theoretical studies on this system have been performed. For example, the recent experimental studies showed the magnitude of MR ratios of 23% [2] and 26% [3] at 4.2 K, and theoretical study based on the Green’s function method showed that a maximum value of the MR ratio was evaluated as 20% [5]. However, except for FM/carbon nanotube/FM junctions [1,2,3,4,5], MR devices with the nanotube were hardly studied so far. If devices with larger MR ratio than the conventional ones can be successfully designed by exploiting characteristic in the nanotube, such the material design will significantly contribute to the development of future nanotube devices.

We therefore aim to propose the novel MR device by focusing on the following characteristic magnetic properties of the nanotube. First, a zigzag nanotube with a finite length appears to have spin-polarized edges, which are qualitatively same as those of a zigzag ribbon [9], because the zigzag nanotube corresponds just to the zigzag ribbon with short periodicity. It was theoretically shown [9] that the zigzag ribbon forms spin polarized states with the ferrimagnetic order along zigzag edges, and the total magnetization of the ribbon is zero. Second, nanotubes encapsulating magnetic atoms such as Fe [10,11], Co, or Ni atoms [12] were recently fabricated.

In this paper, as the novel MR device with the nanotube, we propose “nonmagnetic metal (NM)/zigzag nanotube encapsulating magnetic atoms/NM” junctions. Using the Green’s function technique, we investigate the influence due to the spin-polarized edges and the encapsulated magnetic atoms on the transport. The MR effect due to the direction of spins of magnetic atoms appears reflecting the edges of the nanotube, and the magnitude of the MR ratio becomes much larger than the conventional ones in a certain parameter region.

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2. Model and Method

Figure 1 shows a simplified model, in which the NM has a simple cubic structure, the x -direction of NMs is set to be semi-infinite, and their yz -directions have the periodic boundary condition meaning an infinite system. The number of unit cells in the circumference direction of the nanotube is 15, and the number of zigzag lines [9] is 10. The each edge carbon atom of the nanotube is assumed to interact with its nearest atom of the cubic lattice of the NM.

On the other hand, the encapsulated magnetic atoms have localized spins. We here assume that their spins are divided into several spin clusters which interact with their nearest carbon atoms respectively, and all the spin clusters have the identical total spin. The total spin is approximately represented by a classical spin \mathbf{S} on the assumption that the spin cluster consists of many spins, and further every \mathbf{S} is set to have the same direction. Now, each \mathbf{S} is arrayed along 5-th and 6-th zigzag lines of the nanotube, and it has one to one interaction with carbon atoms in their lines. According to the theory on magnetic impurity problem [13], we take into account antiferromagnetic exchange interactions between conduction electron spins and \mathbf{S} 's, where all the exchange interactions are set to be the same magnitude.

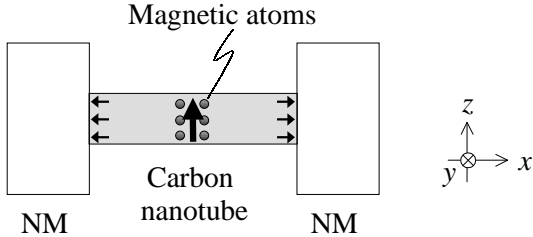


Fig. 1. A schematic illustration of “NM/zigzag carbon nanotube encapsulating magnetic atoms/NM” junctions, where electric currents flow in the x -direction. Arrows at the both edges of the nanotube represent spin-polarized states.

Based on a single orbital Hubbard model with nearest neighbor transfer integrals, the Hamiltonian is given by,

$$H = \sum_i \sum_{\sigma} e_{i,\sigma} c_{i,\sigma}^{\dagger} c_{i,\sigma} + \sum_{\langle i,j \rangle} \sum_{\sigma} (t_{i,j} c_{i,\sigma}^{\dagger} c_{j,\sigma} + \text{h.c.}) + U \sum_{i \in \text{CNT}} n_{i,\uparrow} n_{i,\downarrow}$$

$$-J \sum_{i \in \text{mag}} \sum_{\sigma, \sigma'} \sigma_{\sigma, \sigma'} \cdot \mathbf{S} c_{i,\sigma}^{\dagger} c_{i,\sigma'}, \quad (1)$$

where $c_{i,\sigma}$ ($c_{i,\sigma}^{\dagger}$) is the annihilation (creation) operator of an electron with spin- σ ($=\uparrow$ or \downarrow) at the i -th site, $n_{i,\sigma}$ is the corresponding number operator, $e_{i,\sigma}$ is the corresponding on-site energy, $t_{i,j}$ is the transfer integral between the i -th site and the j -th site, U is the on-site Coulomb energy, and J is the antiferromagnetic exchange integral with negative sign [13]. Furthermore, $\sigma_{\sigma, \sigma'}$ is the (σ, σ') component of the Pauli matrix for the conduction electron spin, and $\mathbf{S} [= (S_x, S_y, S_z)]$ represents the classical spin with $S \equiv |\mathbf{S}|$. Each \mathbf{S} is considered to exist parallel to xz -plane, and an angle between \mathbf{S} and x -axis is written as θ . $\sum_{i \in \text{CNT}} (\sum_{i \in \text{mag}})$ means that the summation is taken for the nanotube (carbon atoms interacting with magnetic atoms).

We treat the term with on-site Coulomb energy within the mean field approximation [9]. Furthermore, in this model, the magnetization of edges of the nanotube is assumed to be pinned parallel to the x -axis, by applying an exchange bias to either the left edge or the right one of the nanotube. The exchange bias is supposed to arise from, for example, magnetic particles attached outside the rim of the nanotube edge.

Using the Green's function technique [14,15], we calculate the conductance at zero temperature,

$$\Gamma(\theta, U) = \sum_{\sigma, \sigma'} \Gamma_{\sigma, \sigma'}(\theta, U), \quad (2)$$

and

$$\Gamma_{\sigma, \sigma'}(\theta, U) = \frac{4\pi^2 e^2}{h} \sum_{i,j,m,n} \langle i, \sigma | \hat{D}_L | j, \sigma \rangle \langle j, \sigma | \hat{T}^{\dagger}(\theta, U) | m, \sigma' \rangle \times \langle m, \sigma' | \hat{D}_R | n, \sigma' \rangle \langle n, \sigma' | \hat{T}(\theta, U) | i, \sigma \rangle, \quad (3)$$

where i, j, m, n are coordinates of contact points in NMs, $\hat{D}_{L(R)}$ is the density-of-states (DOS) operator at the Fermi level E_F of the left NM (right NM), and $\hat{T}(\theta, U)$ is the T -matrix with $G(\theta, U) = (E_F + i0 - H)^{-1}$ and couplings between NMs and the nanotube. Here, $\Gamma_{\sigma, \sigma'}(\theta, U)$ is the conductance for the transmission from the spin- σ state of the left NM to the spin- σ' one of the right NM. Furthermore, we calculate the MR ratio, defined by

$$R_{MR}(\theta, U) = 100 \times \frac{\Gamma(\theta, U) - \Gamma(\pi/2, U)}{\Gamma(\pi/2, U)}. \quad (4)$$

In this calculation, we set $t_{i,j} = t$ (< 0) [16] and $v_{i,j} = 0.1t$, assuming that v is smaller than t because of different types between two orbitals, imperfect lattice matches at the interface, and so

on. The on-site energy of the carbon atom $e_{i,\uparrow}/|t|$ ($=e_{i,\downarrow}/|t|$) is set to be 0 by focusing on its π orbital, and then $e_{i,\uparrow}/|t|$ ($=e_{i,\downarrow}/|t|$) of the both NMs is 5.4 by considering that the s -orbital contributes to the transport of the both NMs. Furthermore, E_F is self-consistently determined so as to keep half filling in the nanotube for the respective parameter sets of U and θ .

3. Calculated Results and Considerations

We first investigate magnetic properties of the carbon nanotube for the finite $U/|t|$ and $JS/|t|=0$. The zigzag nanotube with the finite length forms spin-polarized states with the ferrimagnetic order along zigzag edges, and the total magnetization of the ribbon is zero reflecting an opposite spin polarization between both edges. Such the feature has been seen in the ribbon [9], too. Also, when the spin polarization [17] at the left (right) edge of the nanotube is defined by

$$P_{L(R)} = \frac{D_{L(R),\uparrow} - D_{L(R),\downarrow}}{D_{L(R),\uparrow} + D_{L(R),\downarrow}}, \quad (5)$$

where $D_{L(R),\uparrow}$ is the local DOS at the left (right) edge for the spin- \uparrow at E_F and $D_{L(R),\downarrow}$ is that for the spin- \downarrow at E_F , we obtain $P_L > 0$ and $P_R = -P_L$.

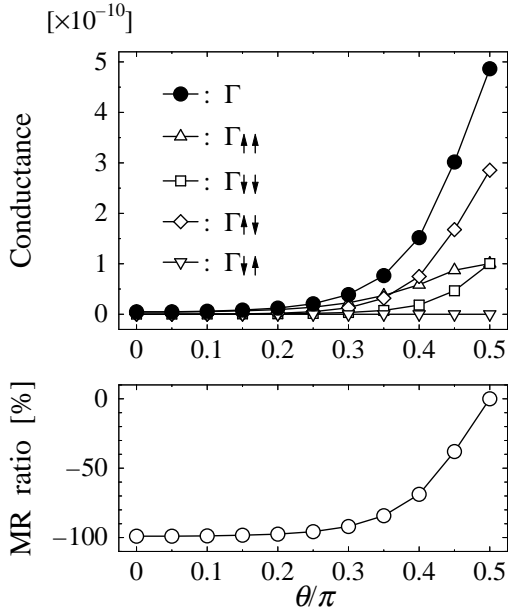


Fig. 2. Upper panel: $\Gamma(\theta, |t|)$ and $\Gamma_{\sigma,\sigma'}(\theta, |t|)$ vs θ . Lower panel: The MR ratio $R_{MR}(\theta, |t|)$ vs θ . The unit of $4\pi^2 e^2/h=1$ is adopted.

In the upper panel of Fig. 2, we show θ dependence of $\Gamma(\theta, U)$ and $\Gamma_{\sigma,\sigma'}(\theta, U)$ with $U/|t|=1$ and

$JS/|t|=-0.5$. When θ is changed from 0 to $\pi/2$, $\Gamma(\theta, |t|)$ increases because of the enhancement of the spin-flip transport. Here, the spin-flip transport is understood by focusing on the main component based on the relations of $P_L > 0$ and $P_R = -P_L$ as follows: First, the spin- \uparrow of the electron from the left edge of the nanotube is flipped by spins of magnetic atoms with $\theta \neq 0$ in the center of the nanotube, and it changes into the spin- \downarrow . Second, the electron flows to the right edge with conservation of the spin. In fact, $\Gamma_{\uparrow,\downarrow}(\theta, |t|)$ rapidly increases with θ , while $\Gamma_{\downarrow,\uparrow}(\theta, |t|)$ has little θ dependence and $\Gamma_{\uparrow,\uparrow}(\theta, |t|)$ and $\Gamma_{\downarrow,\downarrow}(\theta, |t|)$ moderately increase with θ . It should be noted here that such θ dependences are regarded as the MR effect due to the direction of spins of magnetic atoms.

As seen from the lower panel of Fig. 2, $R_{MR}(\theta, U)$ with the same $U/|t|$ and $JS/|t|$ strongly depends on θ owing to the spin-flip transport. We emphasize that the large MR ratio of about 100% can be found between $\theta=0$ and $\pi/2$.

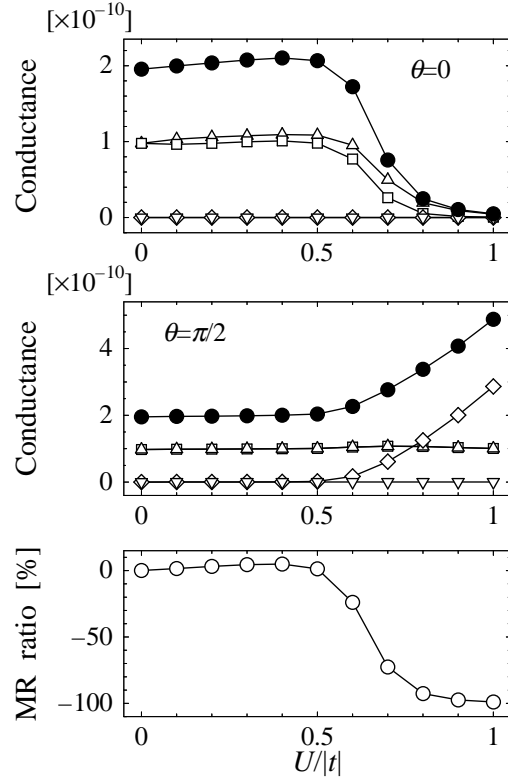


Fig. 3. Upper panel: $\Gamma(0, U)$ and $\Gamma_{\sigma,\sigma'}(0, U)$ vs $U/|t|$. Middle panel: $\Gamma(\pi/2, U)$ and $\Gamma_{\sigma,\sigma'}(\pi/2, U)$ vs $U/|t|$. The meanings of dots in upper and middle panels follow those of the upper panel of Fig. 2. Lower panel: The MR ratio $R_{MR}(0, U)$ vs $U/|t|$. The unit of $4\pi^2 e^2/h=1$ is adopted.

In the upper (middle) panel of Fig. 3, we consider $U/|t|$ dependence of $\Gamma(\theta, U)$ and $\Gamma_{\sigma,\sigma'}(\theta, U)$ with $\theta=0$ ($\theta=\pi/2$) in the case of $JS/|t|=-0.5$. Differ-

ence between $\Gamma(0, 0)$ and $\Gamma(\pi/2, 0)$ is not present. For $U/|t| \leq 0.5$, $\Gamma(0, U)$ and $\Gamma(\pi/2, U)$ have little dependence on $U/|t|$. When $U/|t|$ increases from 0.5, $\Gamma(\pi/2, U)$ increases and $\Gamma(0, U)$ decreases. The behavior indicates that $|P_L|$ and $|P_R|$ increase with increasing $U/|t|$ for $U/|t| > 0.5$ and therefore the spin-flip transport becomes dominant. Note that for $U/|t| > 0.5$, $\Gamma_{\uparrow, \downarrow}(\pi/2, U)$ increases with $U/|t|$, while $\Gamma_{\uparrow, \downarrow}(0, U)$ and $\Gamma_{\downarrow, \uparrow}(0, U)$ decrease with $U/|t|$. Also, the magnitude of $R_{MR}(\theta, U)$ with $\theta=0$ increases with $U/|t|$ for $U/|t| > 0.5$ and becomes about 100% for $U/|t| > 0.8$, although it is very small for $U/|t| \leq 0.5$ (see the lower panel of Fig. 3).

4. Comments

Comparing with conventional FM/carbon nanotube/FM junctions [1,2,3,4,5], we have found that in a certain parameter region, the MR ratio due to the direction of spins of the encapsulated magnetic atoms of the present junctions becomes larger than MR ratios [8] of 9% [1], 23% [2], and 26% [3] of the conventional ones. However, more detailed studies including evaluation of parameters should be necessary in future.

As realistic junctions relevant to the present model, we point out, for example, “Ti/zigzag carbon nanotube encapsulating Fe atoms/Ti” junctions, where zigzag edges of the nanotube are successfully contacted with Ti electrodes. In fact, in the recent experiments, Ti/carbon nanotube/Ti junctions were applied to the field-effect transistor [18], and also carbon nanotubes encapsulating Fe [10,11], Co, or Ni atoms [12] were often fabricated.

5. Conclusion

As the novel MR device with the carbon nanotube, we proposed “NM/zigzag carbon nanotube encapsulating magnetic atoms/NM” junctions. By theoretically investigating the spin-dependent transport, we found that the MR effect due to the direction of spins of magnetic atoms appears reflecting spin-polarized edges of the nanotube. In the case of $U/|t| > 0.8$, the magnitude of the MR ratio becomes about 100%, which is much larger than those of the conventional junctions. We anticipate that such junctions will be applied to magnetic field sensors with high sensitivity.

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